

1-Methoxy-2-propyl acetate
108-65-6 | DTXSID1026796

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 7.33 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.97e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Methoxy-2-propyl acetate</div> <div>Measured: 2.29</div> <div>Predicted: 7.33</div>	<div>Image not found</div> <div>2-(Pyridin-2-yl)ethanol</div> <div>Measured: 28.2</div> <div>Predicted: 35.9</div>	<div>Image not found</div> <div>2-Butoxyethanol</div> <div>Measured: 67.6</div> <div>Predicted: 45.0</div>
<div>Image not found</div> <div>4-Aminobenzoic acid</div> <div>Measured: 316</div> <div>Predicted: 96.6</div>	<div>Image not found</div> <div>Urea, (m-fluorophenyl)-</div> <div>Measured: 58.9</div> <div>Predicted: 59.1</div>	